Accurate Liquid Densities and Near-Critical PVT Behavior for Pure Fluids from Knowledge of Only Z_c and ${}^{\checkmark}$ Using a Simple New Equation of State

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This talk describes a new simple equation of state that accurately predicts liquid densities and PVT behavior near the critical point for both non-polar and polar compounds. By design, the equation also accurately reproduces VLE data for most of the compounds studied. Agreement between experimental and predicted data for isotherms at high reduced pressures, and for vapor pressures and densities, is better for non-polar than for polar compounds. The new equation offers substantial improvements over other modern simple equations of state such as the Peng-Robinson and Dohrn-Prausnitz equations, yet is just as easy to use.

Robustness of the new equation is rooted both in its functional form and in the method of fitting parameters. The equation employs a combination of the Carnahan-Starling repulsive term with a truncated virial-expansion attractive term. Constants and temperature-dependent parameters are derived so as to reproduce the PVT coordinates of the critical point as well as correlations for supercritical PVT data and liquid densities.

A novel approach to VLE due to G.D. Kahl makes use of a temperature-dependent free energy parameter Δ allowing VLE calculations to be performed without lending credibility to the thermodynamic properties of unstable states. In so doing, vapor pressures can be described accurately without adjusting the equation of state itself.

Fitted parameter values are cast in terms of universal, easy-to-use correlations involving only Z_c and \checkmark .

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